

1-Octadecanol
112-92-5 | DTXSID8026935

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.65×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.88×10^{-1}

Confidence level: 7.55×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Terbutylazine

Measured: 1.10×10^{-11}

Predicted: 1.23×10^{-11}

Image not found

2-(2-Butoxyethoxy)ethanol

Measured: 7.44×10^{-11}

Predicted: 5.15×10^{-11}

Image not found

Butane, 1,1'-
[methylenebis(oxy)]bis-

Measured: 3.39×10^{-11}

Predicted: 3.22×10^{-11}

Image not found

Simazine

Measured: 1.10×10^{-11}

Predicted: 1.22×10^{-11}